

2,6-Pyridinedicarboxylic acid, 2-methylhex-3-yl 4-octyl ester

Inchi: InChI=1S/C22H35NO4/c1-6-9-13-17(11-7-2)26-21(24)18-14-10-15-19(23-18)22(25)27-20
InchiKey: PCWBBNHIIAYXCP-UHFFFAOYSA-N
Formula: C22H35NO4
SMILES: CCCCC(CCC)OC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1
Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	5.579		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinpola	2391.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368835&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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